

Fig. 1.

Fig.2.

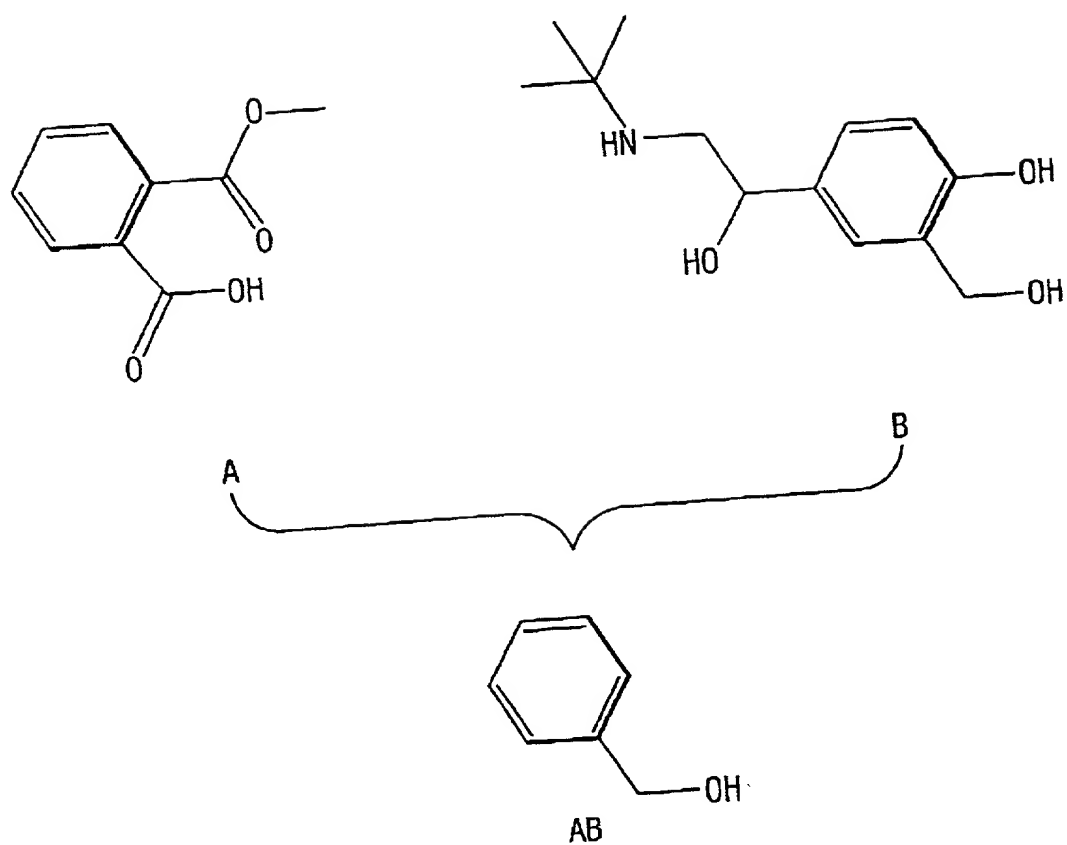


Fig.3.

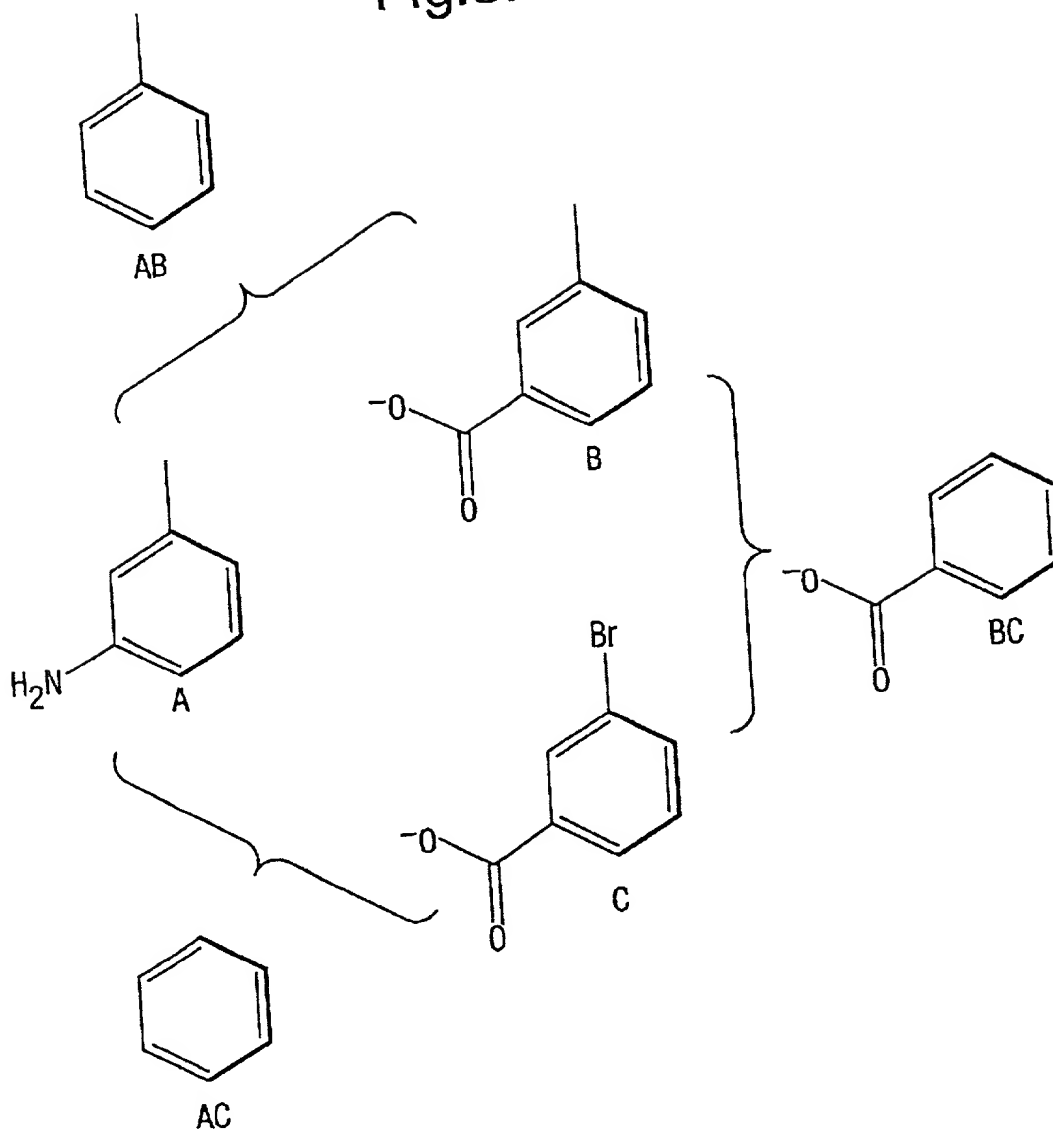


Fig.4.

101 Name	102 Fragment 1	103 Fragment 2	104 Fragment 3	105 Fragment 4	106 Fragment 5	107 Fragment 6	108 ...	109 Molecular Mass	110 Other Descr.	111 Target Property
Acetabulol	4	1	1.8	0	0	0.8	...	336.20984	...	4.545
Acyclovir	1	1	1	0	0	1	...	225.08794	...	3.343
Alprenolol	3	1	0.8	0.857143	0	0.8	...	249.1769	...	-0.121
Amiodarone	5	1	0	0.785714	0.909091	0.8	...	645.02783	...	0.002
Amitriptyline	2	0	0.8	1.64286	0.727273	0	...	266.18192	...	8.765
Amoxicillin	0	0	1.6	1	0	0	...	365.10791	...	5.667
Amphetamine	1	0	0	0.928571	0.818182	0	...	135.10698	...	5.545
Amrinone	0	0	1	0	0	0	...	172.06497	...	1.218
Azathioprine	0	0	0.8	0	0	0	...	277.039	...	-2.269
Azelastine	3	0	0.8	0.928571	0	1.8	...	381.1629	...	3.273
Betaxolol	5	2	0.8	1	0	2.8	...	307.21985	...	7.982
Bisoprolol	4	3	0.8	0.928571	0	0	...	325.23083	...	4.422
Butoralol	2	0	0.8	0.785714	0	0	...	261.17691	...	8.274
Caffeine	0	0	0.8	0	0	0	...	194.08194	...	9.217
...	...	...	...	...	...	...	...	...	...	...